Ab Initio No-Core Shell Model

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1 Introduction

A long-standing goal of nuclear theory is to determine the properties of atomic nuclei based on the fundamental interactions among the protons and neutrons (*i.e.,* nucleons). By adopting nucleon-nucleon (NN), three-nucleon (NNN) and higher-nucleon interactions determined from either meson-exchange theory or QCD, with couplings fixed by few-body systems, we preserve the predictive power of nuclear theory. This foundation enables tests of nature's fundamental symmetries and offers new vistas for the full range of complex nuclear phenomena.

Basic questions that drive our quest for a microscopic predictive theory of nuclear phenomena include:

1. What controls nuclear saturation?

2. How the nuclear shell model emerges from the underlying theory?

3. What are the properties of nuclei with extreme neutron/proton ratios?

4. Can we predict useful cross sections that cannot be measured?

5. Can nuclei provide precision tests of the fundamental laws of nature?

6. Under what conditions do we need QCD to describe nuclear structure?

among others.

Along with other *ab initio* nuclear theory groups, we have pursued these questions [1] with meson-theoretical NN interactions, such as CD-Bonn [2] and Argonne V18 [3], that were tuned to provide high-quality descriptions of the NN scattering phase shifts and deuteron properties. We then add meson-theoretic NNN interactions such as the Tucson-Melbourne [4] or Urbana IX [5] interactions.

More recently, we have adopted realistic NN and NNN interactions with ties to QCD. Chiral perturbation theory within effective field theory (χEFT) [6] provides us with a promising bridge

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[1]present address

between QCD and hadronic systems [7]. In this approach one works consistently with systems of increasing nucleon number [8, 9, 10] and makes use of the explicit and spontaneous breaking of chiral symmetry to expand the strong interaction in terms of a dimensionless constant, the ratio of a generic small momentum divided by the chiral symmetry breaking scale taken to be about 1 GeV/c. The resulting NN and NNN interactions, characterized by the order of the expansion retained (e.g. "next-to-next-to leading order" is NNLO) [11, 12], provide a high-quality fit to the NN data and the A = 3 ground-state (g.s.) properties.

The derivations of NN, NNN, *etc.* interactions within meson-exchange and χEFT are well-established but are not subjects of this review. Our focus is solution of the non-relativistic quantum many-body Hamiltonian that includes these interactions using our no core shell model (NCSM) formalism. In the next section we will briefly outline the NCSM formalism [1, 13] and then present applications, results and extensions in later sections.

2 The *Ab Initio* NCSM Formalism

The *ab initio* NCSM employs realistic interactions, preserves all their symmetries, and treats all A nucleons equally in a basis space of Slater determinants using a single-particle basis, such as the 3D harmonic oscillator (HO) [1, 13]. From this foundation, we show how to derive the well-known standard nuclear shell model, introduced by Maria Goeppert-Mayer and Hans D. Jensen in 1949 (Nobel Prize in physics, 1963), that treats only a small number of valence nucleons outside of inert closed shells. The pathway from the *ab initio* NCSM to the standard shell model involves several major steps that we outline here. In addition, we show that the *ab initio* NCSM combined with the Resonating Group Method (RGM) provides the foundation for microscopic solutions of nuclear reactions with full predictive power.

In the *ab initio* NCSM, we start with the translationally invariant, intrinsic Hamiltonian for all A nucleons. All terms act on relative coordinates – there are no single-particle energies. We then add the HO center-of-mass (CM) Hamiltonian to provide a mean-field potential that improves convergence. The effects of the CM interaction are easily separated and later subtracted. Since realistic NN + NNN interactions are strong at short distances we must introduce a theoretically sound renormalization procedure to render the problem solvable in a basis space with available computer resources. We adopt a renormalization procedure specified by a similarity transformation that softens the interactions and generates effective operators for all observables while preserving all experimental quantities in the low-energy domain. The derived "effective" interactions still act among all A nucleons and preserve all the symmetries of the initial or "bare" NN + NNN interactions. There are two such renormalization procedures that we currently employ, one called the Lee-Suzuki (LS) scheme [14] and the other called the Similarity Renormalization Group (SRG) [15].

For LS renormalization, the infinite HO basis space is divided into a finite model space and an infinite excluded space by the use of projection operators P and Q, respectively. Then the LS effective Hamiltonian H_{eff} is obtained by performing a similarity transformation, X, on the bare Hamiltonian, H, and imposing the decoupling condition $QXHX^{-1}P = 0$; *i.e.,* H_{eff} has no matrix elements between the P and Q spaces, as shown schematically in Fig. 1. Determination of the exact
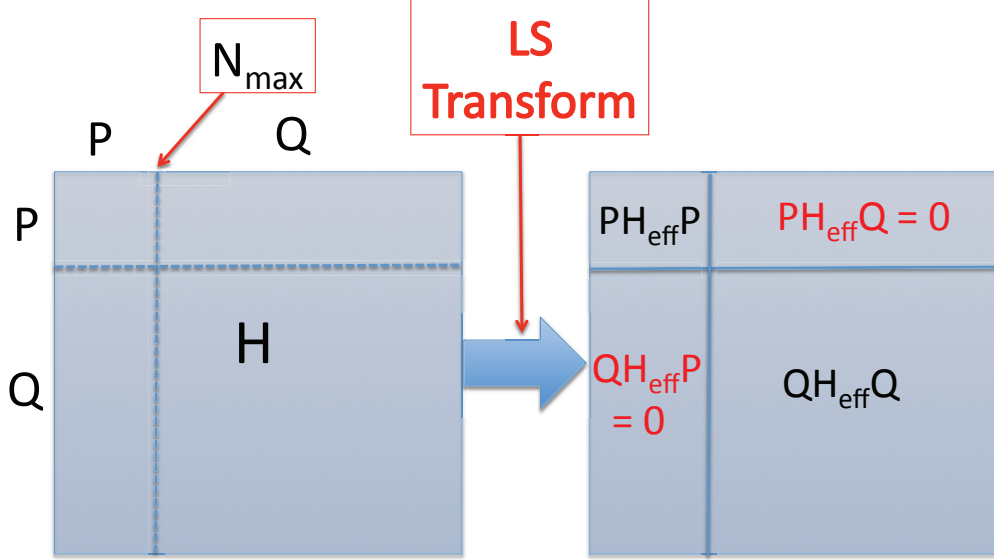
Figure 1: Schematic illustration on how Lee-Suzuki (LS) similarity transformation [14] yields an H_{eff} in a finite model space P decoupled from the infinite complementary Q space.

X requires the solution of the full A-body problem which is not feasible. However, the determination of the A-nucleon H_{eff} from two- or three-body matrix elements, obtained by the solution of the two- or three-body cluster problem, results in an excellent approximation. It also ensures that one recovers the original full problem, if the model space approaches the infinite space, so that the approximation is fully controlled. The LS method can be applied to arbitrary modern NN (NN +NNN) potentials in either coordinate or momentum space.

Recently, we have also adopted the SRG approach [15] for *softening* the NN + NNN interactions. By varying a flow parameter, one can dial down the coupling between the high-energy and low-energy parts of the NN (or NN + NNN) interaction, as illustrated in Fig. 2. These SRG Hamiltonians can be solved in any model space P which is now a simple truncation of the infinite basis SRG Hamiltonian. Figure 3 shows such results for ^4He as a function of the P-space size given in terms of $N_{max}\hbar\Omega$, the maximum HO energy of configurations included above the unperturbed g.s. configuration. The figure clearly shows that the accelerated rate of convergence for the *softer* SRG interactions over the *bare* NN (or NN+NNN) interaction.
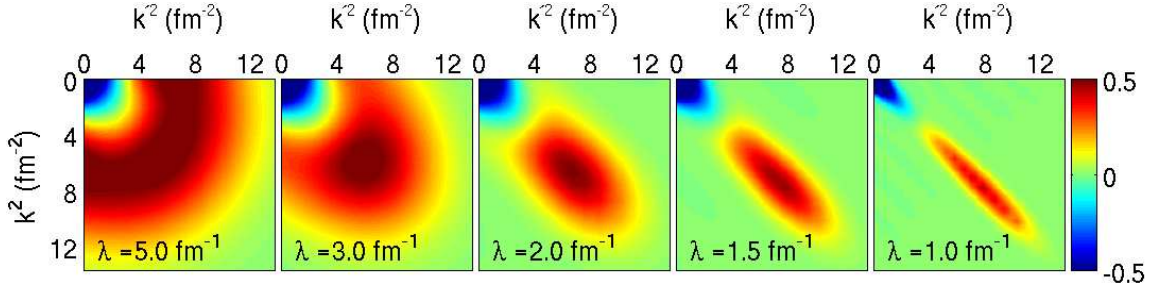
Figure 2: Illustration of how the SRG procedure [15] weakens the strong off-diagonal couplings of an NN potential in momentum space as the flow proceeds to smaller values of λ (left to right panels).

3   NCSM Applications and Results

The results of numerous *ab initio* NCSM applications not only show good convergence with regard to increasing size of the model space P but also have been able to reproduce known properties of $0p$-shell nuclei as well as explain existing puzzles and make predictions of, as yet, unexplained nuclear phenomenon. We list some illustrative examples here.

We display in Fig. 4 the natural-parity excitation spectra of four nuclei in the middle of the $0p-$shell with both the NN and the NN+NNN effective interactions from χEFT [16]. Overall, the NNN interaction contributes significantly to improve theory in comparison with experiment. This is especially well-demonstrated in the odd mass nuclei for the lowest, few excited states. The case of the g.s. spin of ^{10}B and its sensitivity to the presence of the NNN interaction is clearly evident.

A recent calculation has determined the Gamow-Teller (GT) matrix element for the beta decay of ^{14}C, including the effect of NNN forces [17]. These investigations show that the very long lifetime for ^{14}C arises from a cancellation between $0p$-shell NN- and NNN-interaction contributions to the GT matrix element, as shown in Fig. 5. These ^{14}C results were obtained in the largest basis space achieved to date with NNN interactions, $N_{\max} = 8$ ($8\hbar\Omega$) or approximately one billion configurations.

Other noteworthy results include an explanation of the very small quadrupole moment (Q) in ^{6}Li due to a strong cancellation between the one- and two-body contributions to Q [18]. Recent calculations for ^{12}C explained the measured ^{12}C B(M1) transition from the g.s. to the $(1^{+}, 1)$ state at 15.11 MeV and showed more than a factor of 2 enhancement arising from the NNN interaction. Neutrino elastic and inelastic cross sections on ^{12}C were shown to be similarly sensitive to the NNN interaction and their contributions significantly improve agreement with experiment [19]. Working in collaboration with experimentalists, we uncovered a puzzle in the GT-excited state strengths in A=14 nuclei [20]. Its resolution may lie in the role of intruder-state admixtures, but this will require further work.

4   Extensions of the NCSM for treating heavier mass nuclei

The basic idea of the *ab initio* Shell Model with a Core [21] is to use the well-established *ab initio* NCSM to solve for the core and one- and two-body terms that are needed for performing standard
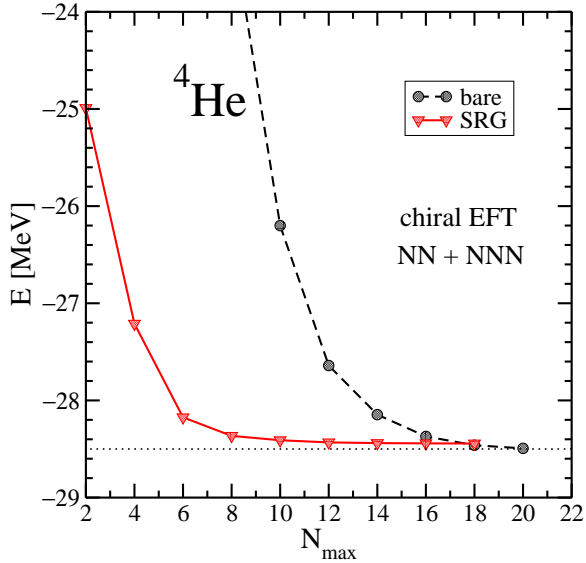
Figure 3: Convergence of the ^4He g.s. energy with the size of the HO basis. Calculations with the bare (dashed line) and the SRG evolved (solid line) χEFT NN+NNN interactions are compared. The SRG evolution parameter $\lambda = 2$ fm^{-1} was used (see Fig.2). The dotted line denotes the extrapolated g.s. energy (-28.5 MeV), which is close to the experiment (-28.3 MeV).

Shell Model (SSM) calculations for nuclei in the sd- and pf-shells. Such SSM calculations can be performed in vastly smaller model spaces than those required for converged NCSM calculations.

For illustration let us consider $0p$-shell nuclei. We first perform a standard *ab initio* NCSM calculation to obtain *converged* eigenenergies and eigenfunctions for the $A = 6$ system, *e.g.,* ^{6}Li. Next, we carry out a unitary transformation of these ^{6}Li results into the smaller model space of $0\hbar\Omega$ excitations, which is equivalent to a neutron and a proton in the $0p$-shell and the other four nucleons *energetically frozen* in the $0s$-shell. Thus, we obtain *only* two-body matrix elements in the $0p$-shell, although we started with a full solution of the $A = 6$ system in the NCSM approach. However, these two-body matrix elements contain *all* the physics of the six-nucleon system. These two-body matrix elements can be separated into a core and one- and two-body components suitable for SSM calculations. In a similar manner we can calculate the seven-body cluster in the $0p$-shell by performing an *ab initio* NCSM calculation for ^{7}Li and transforming this result into the $0p$-shell. In this case, we can also determine the three-body term in the $0p$-shell. These core and one-, two- and three-body terms can then be used to perform SSM calculations for all the nuclei in the $0p$-shell, in much smaller model spaces. Effects of neglected four-body interactions appear to be small.

The *same* approach, outlined previously for obtaining the effective components of the shell-model Hamiltonian in a single major shell, *e.g.,* the $0p$-shell, can also be utilized for computing the effective components of any physical operator in the same major shell. See Ref.[18] for details. The results of such calculations for the quadrupole moment (Q) of ^{6}Li are illustrated in Fig. 6. Clearly, the very small Q-moment for ^{6}Li arises from complex many-body correlations among all six nucleons,
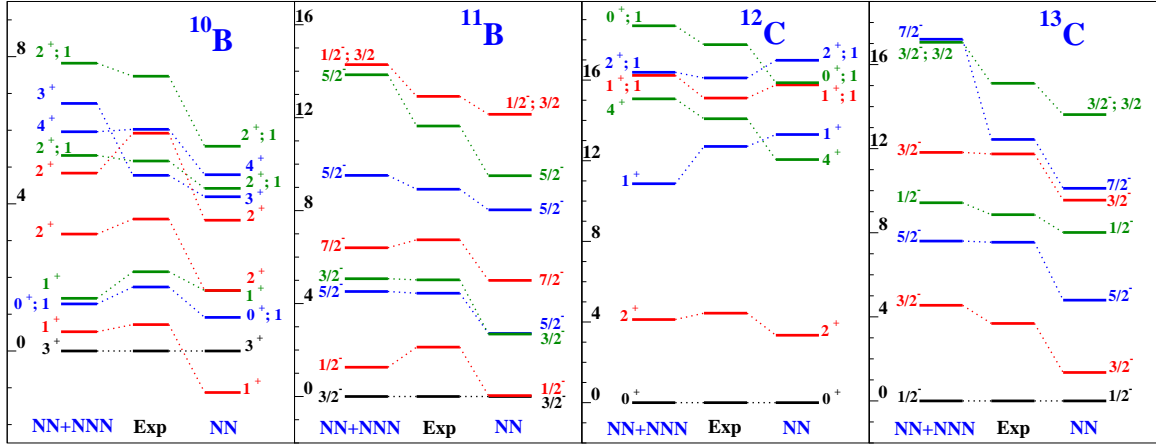
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Figure 4: States dominated by $0p$-shell configurations for ^{10}B, ^{11}B, ^{12}C, and ^{13}C calculated at $N_{\max} = 6$ using $\hbar\Omega = 15$ MeV (14 MeV for ^{10}B). Most of the eigenstates are isospin T=0 or $1/2$, the isospin label is explicitly shown only for states with T=1 or $3/2$. The excitation energy scales are in MeV (adopted from Ref [16]).

leading to a large cancellation between the one- and two-body contributions.

The above $0p$-shell results encourage us to extend this approach to nuclei in the sd-shell, which will require converged results for nuclei with $A = 16, 17, 18$ and 19. In this regard we are working on a new version of the Importance Truncation approach of Roth [22] to obtain these results.

5   Applications to nuclear reactions

A realistic *ab initio* description of light nuclei with predictive power must have the capability to describe all bound and unbound states within a unified framework. *Ab initio* calculations for scattering processes involving more than four nucleons overall are challenging and still a rare exception [23]. Even calculations of resonant states are quite complicated [24]. The development of an *ab initio* theory of low-energy nuclear reactions on light nuclei is key to further refining our understanding of the fundamental nuclear interactions among the constituent nucleons and providing, at the same time, accurate predictions of crucial reaction rates for nuclear astrophysics.

A fully *ab initio* approach to nuclear reactions based on the NCSM requires a more precise treatment of the wave-function asymptotics and the coupling to the continuum. Therefore, we have developed a new approach, the *ab initio* NCSM/RGM [25, 26], capable of simultaneously describing both bound and scattering states in light nuclei, by combining the resonating-group method (RGM) [27] with the *ab initio* NCSM. The RGM is a microscopic cluster technique based on the use of A-nucleon Hamiltonians, with fully anti-symmetric many-body wave functions built assuming that the nucleons are grouped into clusters. By combining the NCSM with the RGM, we complement the ability of the RGM to deal with scattering and reactions with the utilization of realistic interactions and a consistent microscopic description of the nucleonic clusters achieved via *ab initio* NCSM,
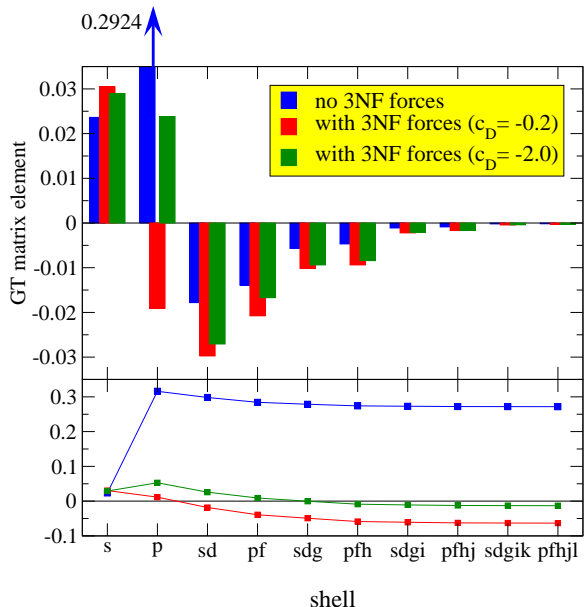
Figure 5: Contributions to the ^{14}C beta decay matrix element as a function of HO shell when the nuclear structure is described by the χEFT interaction (adopted from Ref. [17]). Top panel displays the contributions with (two right bars of each triplet) and without (leftmost bar of each triplet) the NNN force at $N_{\max} = 8$. Contributions are summed within each shell to yield a total for that shell. The bottom panel displays the running sum of the GT contributions over the shells. Note the order-of-magnitude suppression of the $0p$-shell contributions arising from the NNN force.

while preserving important symmetries, including the Pauli exclusion principle and translational invariance.

Using the above NCSM/RGM formalism, we performed extensive nucleon-^{4}He calculations with the SRG-evolved NN potentials. The agreement of our calculated n-^{4}He and p-^{4}He phase shifts with the experimental ones is quite reasonable for the S-wave, D-wave and $^2P_{1/2}$-wave. The $^2P_{3/2}$ resonance is positioned at higher energy in the calculation and the corresponding phase shifts are underestimated with respect to the experimental results, although the disagreement becomes less and less pronounced beyond the resonance energy. The observed difference is largely due to a reduction in spin-orbit strength caused by the neglect of the NNN interaction in our calculations. More details are given in Ref. [28]. For energies beyond the $^2P_{3/2}$ resonance, our calculations compare favorably with the experimental data. This is shown in Fig. 7, where the NCSM/RGM p-^{4}He results are compared to various experimental data sets [29, 30, 31, 32] in the energy range $E_p \sim 12 - 17$ MeV.

The ^{7}Be$(p,\gamma)^8$B capture reaction plays a very important role in nuclear astrophysics as it serves as an input for understanding the solar neutrino flux [33]. The extrapolation of the S-factor (i.e., the cross section divided by the Gamow factor) to astrophysically relevant energies relies on nuclear theory. We performed NCSM/RGM calculations of the p-^{7}Be scattering as a necessary preparatory step to investigate the ^{7}Be$(p,\gamma)^8$B capture reaction [28]. In the calculation presented in Fig. 8 that
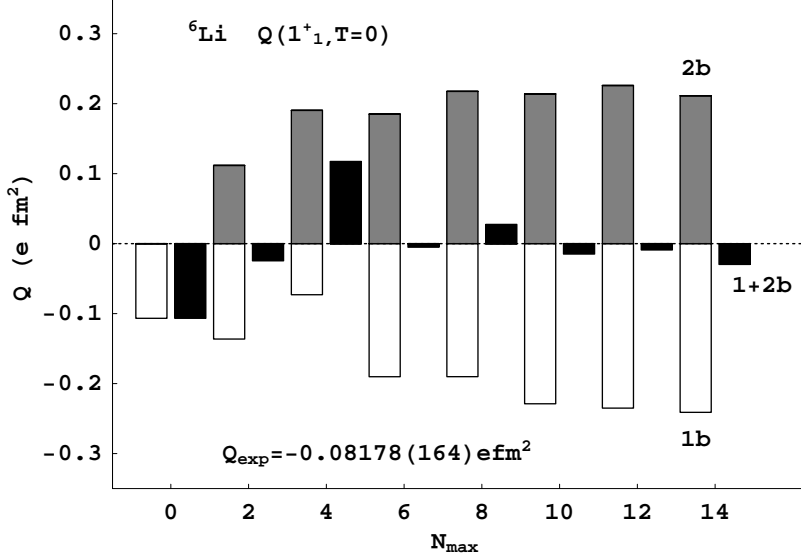
Figure 6: The quadrupole moment (Q) of the g.s. for ^{6}Li [1^+(T=0) is shown in terms of one- and two-body contributions, as a function of increasing model-space size. The one- and two-body contributions and total Q are depicted as white, gray and black histograms, respectively [18].

included the g.s. and the lowest four excited states of ^{7}Be we found a 2^+ state bound by 0.16 MeV corresponding to the ^{8}B ground state. In experiment, ^{8}B is bound by 137 keV [34]. The calculated lowest 1^+ resonance appears at about 0.7 MeV. It corresponds to the experimental ^{8}B 1^+ state at $E_x = 0.77$ MeV. This resonance dominates the inelastic cross section as seen in the left part of Fig. 8. We find a 0^+, another 1^+ and two 2^+ resonances not included in the current ^{8}B evaluation [34]. We note, however, that in the very recent Ref. [35], the authors claim the observation of low-lying 0^+ and 2^+ resonances, based on an R-matrix analysis of their p-^{7}Be scattering experiment. Effects of the 0^+, the second 1^+ and the second 2^+ states are visible in the inelastic cross section above the first 1^+ state resonance. On the other hand, the 3^+ resonance affects, in particular, the elastic cross section. Calculations of the ^{7}Be$(p,\gamma)^8$B capture within the NCSM/RGM are in progress.

The deuterium-tritium reaction is important for possible future fusion energy generation. Even though it has been well studied experimentally, its first principles theoretical understanding is important. The ^{3}H$(d,n)^4$He and its mirror reaction ^{3}He$(d,p)^4$He are also of interest for understanding primordial nucleosynthesis. In addition, the ^{3}He$(d,p)^4$He is one of the few reactions to present strong electron screening effects. The first *ab initio* calculations for these reactions within the NCSM/RGM framework are under way. Our first results were obtained with the SRG NN interaction with $\lambda = 1.5$ fm^{-1}, for which the resonance energies are close to experimental values [36]. The astrophysical S-factor for the ^{3}He$(d,p)^4$He reaction from beam-target experiments is compared to NCSM/RGM calculations for bare nuclei in the right panel of Fig. 8. We observe a slightly different shape of the peak than that suggested by the "Trojan-horse" data from Ref. [37]. Also, no low-energy enhancement is present in the theoretical results contrary to the beam-target data of Ref. [38] affected by
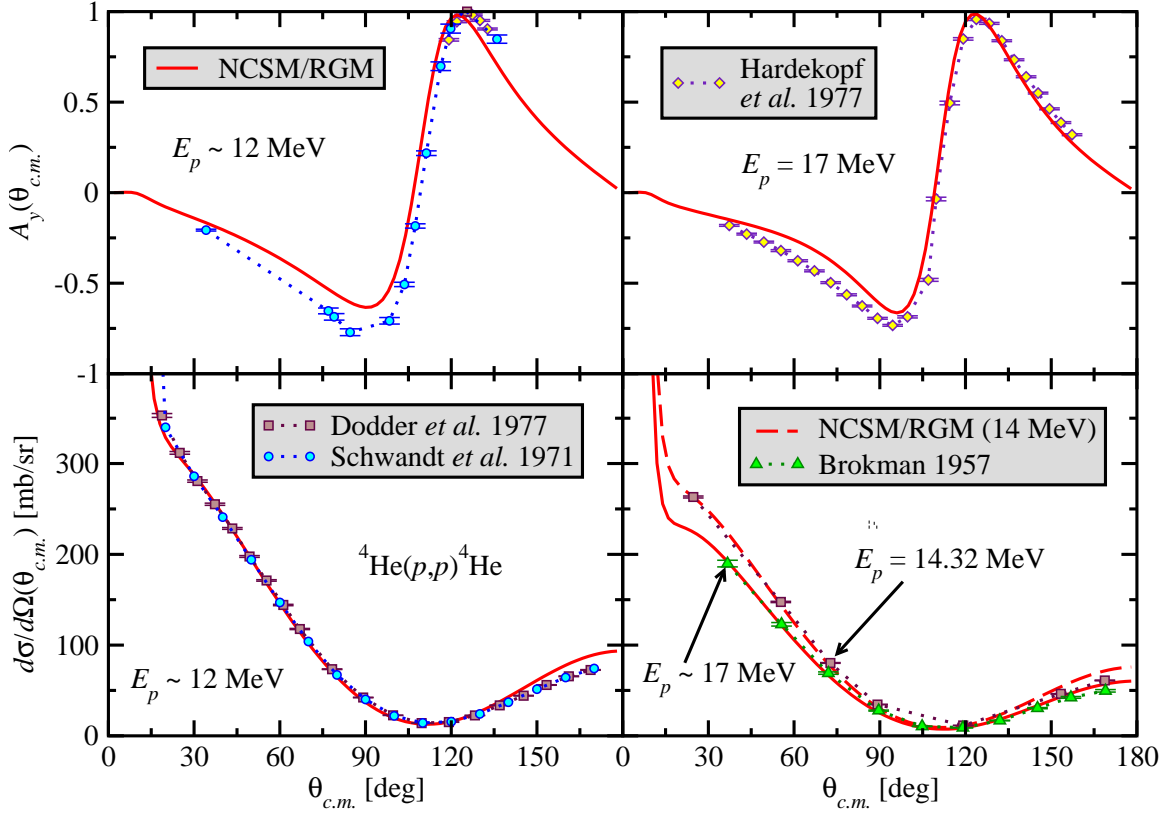
Figure 7: Calculated p-^{4}He differential cross section (bottom panels) and analyzing power (top panels) for proton laboratory energies $E_p = 12, 14.32$ and 17 MeV compared to experimental data from Refs. [29, 30, 31, 32]. The SRG-N^{3}LO NN potential with $\lambda = 2.02$ fm^{-1} was used.

the electron screening.

6   Summary and Outlook

The *ab initio* NCSM treats all A nucleons equally with modern NN+NNN interactions and successfully describes properties of nuclei throughout the $0p$-shell. In combination with the RGM, it provides a truly microscopic approach for nuclear reactions. Several investigations are underway to extend the *ab initio* NCSM to nuclei with $A > 16$ and to more completely unify the original *ab initio* NCSM with the NCSM/RGM approach. The outlook includes, but is not limited to:

1. Development of effective NN, NNN and even NNNN interactions for more detailed investigations of $0p$- and sd-shell nuclei.

2. Development of symmetry-adapted basis spaces such as SU(3) [39].

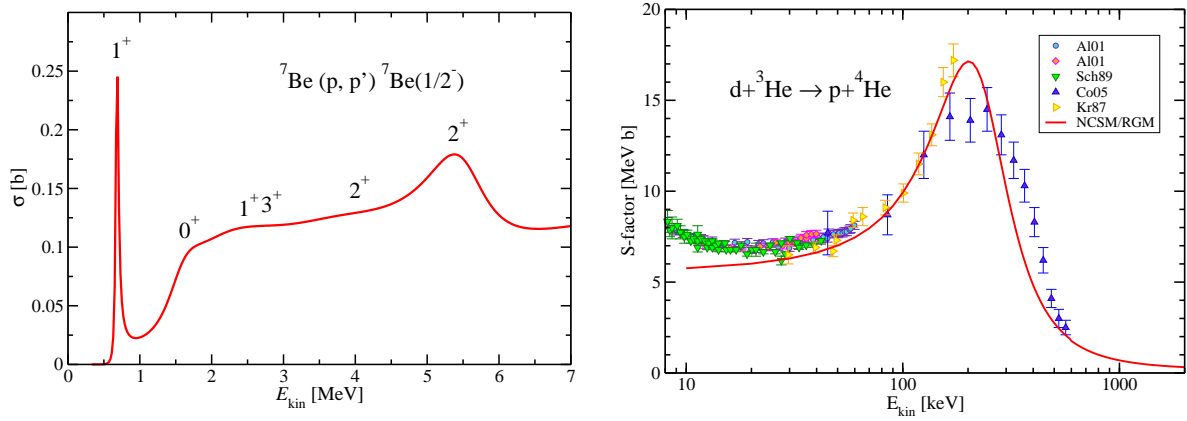3. Extension of the NCSM calculations to sd- and pf-shell nuclei, *i.e.*, *ab initio* SM with a core.

Figure 8: Calculated inelastic $^7\mathrm{Be}(p,p')^7\mathrm{Be}(1/2^-)$ cross section with indicated positions of the P-wave resonances (left figure). Calculated S-factor of the $^3\mathrm{He}(d,p)^4\mathrm{He}$ fusion reaction compared to experimental data (right figure). Energies are in the center of mass. The SRG-N^{3}LO NN potential with $\lambda = 1.85$ fm^{-1} ($\lambda = 1.5$ fm^{-1}) was used, respectively.

4. Extension of the NCSM/RGM approach to nuclear reactions with more massive projectiles and three-cluster final states

5. Coupling of the binary-cluster $(A-a, a)$ NCSM/RGM basis and the standard A-nucleon NCSM basis to unify the original *ab initio* NCSM and NCSM/RGM approaches. This will result in an optimal and balanced description of both bound and unbound states. We name this approach *ab initio* NCSM with the continuum (NCSMC).

6. Improved extrapolation techniques for estimating converged results.

7. The development of new techniques for quantifying theoretical uncertainties.

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